Quasi-Homogeneous Dynamical Structure Factor for Atomic-Trap Bose Condensates

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Abstract

The essence of the Thomas-Fermi model is the assumption that the local behavior of a many-body system can be approximated by that of a homogeneous system. In this paper, we present the natural extension of the static Thomas-Fermi treatment of dilute Bose condensates, by describing the dynamical behavior of the condensate in the same quasi-homogeneous approximation. In particular, we calculate the dynamical structure factor $S(\mathbf{q},\omega)$ of a low-temperature condensate, confined in a harmonic oscillator trap. The result is a remarkably simple analytical function, which, with the proper interpretation, gives a powerful and insightful description of the scattering properties of the BEC-system.

I. INTRODUCTION

The achievement [1]– [3] of the long-elusive [4] goal of atomic Bose-Einstein condensation has set the stage for exciting applications, such as tests of fundamental mean-field theories [5] and the atom laser [6]. The engineering problems associated with most applications are generally less severe if the condensate is highly populated and it might be necessary to create 'larger' condensates before a practical use of atomic-trap BEC can be demonstrated. Regarding this point, we note that recent experiments (see for example Ref. [7]) report a significant increase in number of condensed atoms. Thus, the 'large condensate' or 'Thomas-Fermi' limit, aside from its convenient simplicity, is also of great importance from a practical point of view.

The essence of the Thomas-Fermi model is the 'quasi-homogeneous picture', which is the assumption that the behavior of a condensate near a position $\mathbf{r}$, can be approximated by that of a homogeneous BEC with chemical potential equal to the local effective chemical potential:

$$\mu(\mathbf{r}) = \mu_T - V(\mathbf{r}), \tag{1}$$

where μ_T is the chemical potential of the trapped condensate and $V(\mathbf{r})$ the trapping potential. Although many authors [8]– [17] have explored the physics and the limits of this description, most efforts have been limited to the static description of a dilute BEC. In fact, the few studies that have calculated dynamical properties [16]– [17] starting from a Thomas-Fermi description, have gone beyond the quasi-homogeneous picture in order to obtain a discrete spectrum. This allowed the description of interesting effects due to the finite size of the system, but caused the formalism to lose some of the simplicity of the straightforward quasi-homogeneous description. Perhaps, the inability of the quasi-homogeneous description to calculate such finite-size effects is to be blamed for the lack in the literature of a simple quasi-homogeneous treatment of the dynamical BEC structure.

In this paper, we present such treatment, and investigate the limits and restrictions inherent to the model. The simplicity of the results, combined with a proper understanding

of the limits, gives a powerful formalism that can be used to interpret experimental data, as well as to check certain limits of more complicated computational schemes. Furthermore, the insight gained from studying the limits of validity, indicates how experimental data taken from a finite-size system can be interpreted in terms of the homogeneous system.

The quantity that we choose to calculate is the dynamical structure factor, which represents the information content of non-resonant scattering data about the dynamical many-body structure of the scattering system. More relevant to the atomic-trap BEC-systems, resonant light scattering gives a cross-section which in the off-resonant limit is also proportional to the dynamical structure factor [19], [20], [21]. More precisely, the single-scattering differential cross section $d^2\sigma/d\Omega d\omega$, where $d\Omega$ is an infinitesimal solid angle and ω the energy transfer ($\hbar = 1$ in our units), is equal to

$$\frac{d^2\sigma}{d\Omega\ d\omega} = |f(\mathbf{q})|^2 S(\mathbf{q},\omega)\ , \tag{2}$$

where $\mathbf{q}$ is the momentum transfer, $S(\mathbf{q},\omega)$ the dynamical structure factor of the many-body scattering system, and $f(\mathbf{q})$ the scattering length that describes the scattering of an incident particle by an individual target particle. For non-resonant scattering, the scattering length can depend explicitly on the momentum transfer, whereas for off-resonant light scattering the scattering length is the large-detuning limit of the usual single-atom resonant scattering length ($\sim \lambda\gamma/\Delta$, where λ is the inverse of the resonant wave number, γ the width of the excited resonant state and Δ the detuning of the incident light).

The structure factor is the Fourier-transform of the density-density correlation function,

$$S(\mathbf{q},\omega) = (2\pi)^{-1} \int d^3x\ d^3x' dt'\ \exp\left[-i\mathbf{q}\cdot(\mathbf{x}'-\mathbf{x}) - \omega t'\right]\ \langle\hat{\rho}(\mathbf{x}',t')\hat{\rho}(\mathbf{x},0)\rangle\ \ , \tag{3}$$

where $\hat{\rho}$ represents the density operator and $\langle\ \rangle$ denotes the thermally averaged expectation value. A substitution of the spatial integration variables in (3) to sum and difference variables, $\mathbf{R} = [\mathbf{x}+\mathbf{x}']/2$ and $\mathbf{r} = \mathbf{x}'-\mathbf{x}$, gives

$$S(\mathbf{q},\omega) = \int d^3R\ \sigma(\mathbf{R};\mathbf{q},\omega)$$

$$\text{where}\ \ \sigma(\mathbf{R};\mathbf{q},\omega) = (2\pi)^{-1} \int \mathrm{d^3r\ dt'}\ \exp\left[-\mathrm{i}(\mathbf{q}\cdot\mathbf{r} - \omega\mathrm{t}')\right] \langle\hat{\rho}(\mathbf{R}+\mathbf{r}/2,\mathrm{t}')\hat{\rho}(\mathbf{R}-\mathbf{r}/2,0)\rangle \tag{4}$$

is a dynamical structure factor density. In the quasi-homogeneous approximation, we replace the correct structure density by $\sigma^{(\mathrm{hom})}_{\mu(\mathbf{R})}(\mathbf{q},\omega)$, its value for a homogeneous system of chemical potential $\mu(\mathbf{R})$:

$$S(\mathbf{q},\omega) \approx S_{TF}(\mathbf{q},\omega) = \int d^3R\, \sigma^{(\mathrm{hom})}_{\mu(\mathbf{R})}(\mathbf{q},\omega) \quad , \tag{5}$$

which leads to an analytical expression, as we show below.

II. HOMOGENEOUS BEC IN THE BOGOLIUBOV APPROXIMATION

In treating a homogeneous system, the natural choice for a single-particle basis is the set of plane wave states, labeled by their wave vector/momentum $\mathbf{k}$. Describing the interparticle interaction in the shape-independent approximation by means of a scattering length a, the second-quantized Hamiltonian operator reads

$$\hat{H} = \sum_{\mathbf{k}} (k^2/2m - \mu) c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + \frac{\lambda}{2V} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}} c^\dagger_{\mathbf{k}'-\mathbf{q}} c_{\mathbf{k}'} c_{\mathbf{k}} \tag{6}$$

where we have included the chemical potential μ, $\lambda = 4\pi a/m$, V denotes the macroscopic volume of the system, and $c, c^\dagger$ represent the annihilation and creation operators.

For the purpose of describing the static properties of a BEC of N atoms with a coherent condensate of an average of N_0 atoms in the $\mathbf{k} = 0$-mode, we can replace $c_{\mathbf{k}=0}$ and $c^\dagger_{\mathbf{k}=0}$ by $\sqrt{N_0}$. Provided the depletion is low, $(N - N_0)/N \ll 1$, we can neglect terms that contain less than two factors of $\sqrt{N_0}$. In this approximation, only valid for dilute ($na^3 \ll 1$) and low temperature Bose condensates ($k_B T < \lambda n_0$, where n_0 is the condensate density, $n_0 = N_0/V$, T the temperature and k_B the Boltzmann constant), the hamiltonian is phonon-like:

$$\begin{aligned} \hat{H} \approx V\, (-\mu n_0 + \frac{\lambda}{2} n_0^2) + \sum_{\mathbf{k}\neq 0} (k^2/2m - \mu + n_0\lambda) c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \; + \\ n_0\lambda \sum_{\mathbf{k}\neq 0} \frac{\left(c^\dagger_{\mathbf{k}} + c_{-\mathbf{k}}\right)}{\sqrt{2}} \frac{\left(c^\dagger_{-\mathbf{k}} + c_{\mathbf{k}}\right)}{\sqrt{2}} \quad . \end{aligned} \tag{7}$$

The free energy of the system, F, also contains the entropy, which we denote by S, and F is equal to [22] $F = \langle \hat{H} \rangle - TS$.

To lowest order, consistent with the assumption of low depletion, we can approximate the expectation value of $\hat{H}$ by the first term of (7)

$$\langle \hat{H} \rangle \approx V \left(-\mu n_0 + \frac{\lambda}{2} n_0^2 \right) \ , \tag{8}$$

and determine the chemical potential by minimizing F with respect to n_0, giving

$$\mu \approx n_0 \lambda \ . \tag{9}$$

To determine expectation values involving non-zero wavenumbers, we return to (7) with (9). In doing so, we also find it useful to introduce Hermitian operators

$$\begin{aligned} \Phi_{\mathbf{k}} &= \frac{\left(c_{-\mathbf{k}} + c_{\mathbf{k}}^{\dagger} \right)}{\sqrt{2}} \ , \\ \Pi_{\mathbf{k}} &= \frac{\left(c_{\mathbf{k}} - c_{-\mathbf{k}}^{\dagger} \right)}{i\sqrt{2}} \ , \end{aligned} \tag{10}$$

which represent the fluctuations of the density and velocity field [23]. The canonical boson commutator relations such as $\left[c_{\mathbf{k}}^{\dagger}, c_{\mathbf{k}'} \right] = \delta_{\mathbf{k},\mathbf{k}'}$, are equivalent to the requirement that $\Phi_{\mathbf{k}}$ and $\Pi_{\mathbf{k}}$ are canonically conjugate: $[\Phi_{\mathbf{k}}, \Pi_{\mathbf{k}'}] = i\delta_{\mathbf{k},\mathbf{k}'}$. With the fluctuation operators the Hamiltonian takes on the following form:

$$\hat{H} = \sum_{\mathbf{k}} (k^2/2m) \frac{1}{2} (\Phi_{\mathbf{k}} \Phi_{-\mathbf{k}} + \Pi_{-\mathbf{k}} \Pi_{\mathbf{k}}) + \mu \Phi_{\mathbf{k}} \Phi_{-\mathbf{k}} \quad . \tag{11}$$

In obtaining (11), we have neglected a constant term, unimportant in describing the behavior of the system.

At this point, we invoke the quasi-particle concept and introduce quasi-particle fluctuation operators $\Phi_{\mathbf{k}}^{'}, \Pi_{\mathbf{k}}^{'}$, defined as in (10) with the particle creation and annihilation operators replaced by quasi-particle creation and annihilation operators. We cast the Bogoliubov transformation between particle and quasi-particle operators in terms of the fluctuation operators. It can be seen that this transformation cannot mix Π and Φ operators because of time reversal symmetry. Indeed, the density fluctuation expectation value of a time-reversed state is equal to the expectation value of the state, whereas the expectation value of the

velocity-field fluctation changes sign. The only transformation that preserves canonicity is then a simple 'scaling' transformation:

$$\begin{aligned} \Phi_{\mathbf{k}} &= \alpha_{\mathbf{k}} \ \Phi'_{\mathbf{k}} \ , \\ \Pi_{\mathbf{k}} &= \alpha_{\mathbf{k}}^{-1} \ \Pi'_{\mathbf{k}} \ , \end{aligned} \tag{12}$$

which is the Bogoliubov transformation in fluctuation operator notation. We choose α real so that all Φ and Π-operators are Hermitian. In addition, the isotropical nature of the system suggests that the scaling parameter $\alpha_{\mathbf{k}}$ should only depend on the magnitude of the momentum, $\alpha_{\mathbf{k}} = \alpha_k$. The value of the scaling parameter is determined by minimizing the free energy with respect to α_k. In computing the expectation value of the hamiltonian operator, the temperature average of the fluctuation correlations depend on the quasi-particle occupation numbers ν_k, $\langle \Pi'_{\mathbf{k}} \Pi'_{-\mathbf{k}} \rangle = \langle \Phi'_{-\mathbf{k}} \Phi'_{\mathbf{k}} \rangle = (1 + 2\nu_k)/2$:

$$\frac{\partial F}{\partial \alpha_k} = \frac{\partial}{\partial \alpha_k} \left[\left[\frac{1}{2} (\alpha_k^2 + \alpha_k^{-2})(k^2/2m) + \mu \alpha_k^2 \right] \ \frac{(1 + 2\nu_k)}{2} \ \right] = 0 \ , \tag{13}$$

although the occupation numbers cancel out in optimizing α_k and we find

$$\alpha_k^2 = \frac{k^2/2m}{E_k} \ , \tag{14}$$

where E_k denotes the usual Bogoliubov dispersion relation, $E_k = \sqrt{(k^2/2m + \mu)^2 - \mu^2}$. Unlike α_k, expectation values of observable quantities do depend on the quasi-particle occupation numbers $\nu_k = (\exp[\beta E_k] - 1)^{-1}$. In the last line of (14) we display the square of the scaling parameter, because α^2 is the quantity that appears in the expression for the dynamical structure factor, $\langle \hat{\rho}_{-\mathbf{q}} \hat{\rho}_{\mathbf{q}} \rangle \approx n_0^2 \delta_{\mathbf{q},0} + n_0 \langle \Phi_{-\mathbf{q}} \Phi_{\mathbf{q}} \rangle \ = n_0^2 \delta_{\mathbf{q},0} + n_0 \alpha_q^2 \langle \Phi'_{-\mathbf{q}} \Phi'_{\mathbf{q}} \rangle$. Consequently, we find for the dilute homogeneous BEC of low depletion, the following expression for the dynamical structure factor density:

$$\begin{aligned} \sigma_\mu^{(\mathrm{hom})}(\mathbf{q}, \omega) &\approx \alpha_q^2 n_0 \ (2\pi)^{-1} \int dt' \exp(i\omega t') \langle \Phi'_{-\mathbf{q}}(t') \Phi'_{\mathbf{q}}(0) \rangle \\ &= \frac{q^2/2m}{E_q} \ n_0 \left[(1 + \nu_q) \delta(\omega - E_q) + \nu_q \ \delta(\omega + E_q) \right] \ , \end{aligned} \tag{15}$$

which is the low-temperature generalization of the well-known zero-temperature result [24]. Note that the dependence on the occupation numbers of (15) is reminiscent of stimulated and spontaneous photon emission.

III. THOMAS-FERMI DYNAMICAL STRUCTURE FACTOR

We calculate the structure factor $S(\mathbf{q},\omega)$ in the quasi-homogeneous approximation (5), using the above derived result (15) for the homogeneous BEC. In this manner we find

$$\begin{aligned} S_{TF}(\mathbf{q},\omega) &= \int d^3R \;\; \sigma^{(\mathrm{hom})}_{\mu(\mathbf{R})}(\mathbf{q},\omega) \\ &= \int d^3R \, n_0(\mathbf{R}) \, \frac{q^2/2m}{\omega} \left[[1+\nu_q(\mathbf{R})] \, \delta\left(\omega - E_q(\mathbf{R})\right) - \nu_q(\mathbf{R}) \delta\left(\omega + E_q(\mathbf{R})\right) \right] \;, \end{aligned} \tag{16}$$

where the position dependence of $\omega_q(\mathbf{R})$ and $\nu_q(\mathbf{R})$, defined as

$$\begin{aligned} E_q(\mathbf{R}) &= \sqrt{\left(q^2/2m + \mu(\mathbf{R})\right)^2 - \mu^2(\mathbf{R})} \;\; , \\ \nu_q(\mathbf{R}) &= \frac{1}{\exp\left[\beta E_q(\mathbf{R})\right] - 1} \; , \end{aligned} \tag{17}$$

stems from the $\mathbf{R}$-dependence of the effective chemical potential $\mu(\mathbf{R})$. We remark that in the quasi-homogeneous description, the phonon-like (or collective mode-like) delta-peak in the spectrum (16), implies that the energy and momentum transfer, ω and q, determine the spatial condensate region that is probed: the positions $\mathbf{R}$ for which $E_q(\mathbf{R}) = \omega$.

We perform the spatial integration of Eq.(16) for the simple example of a spherically symmetric harmonic oscillator trap with potential $V(R)$,

$$V(R) = \frac{\omega_T}{2}(R/L)^2 \; , \tag{18}$$

where ω_T is the trap frequency and L the extent of its single-particle ground-state, $L = 1/\sqrt{m\omega_T}$. The Thomas-Fermi expression for the condensate density in the low-depletion limit is easily obtained from the homogeneous result, $\lambda n_0 \approx \mu$ (9), which gives the following quasi-homogeneous expression for the condensate density $n_0(\mathbf{R})$:

$$n_0(\mathbf{R}) = \frac{\mu(\mathbf{R})}{\lambda} = \frac{[\mu_T - V(\mathbf{R})]}{\lambda} \theta(R - R_0) \; . \tag{19}$$

The condensate radius R_0 ($V(R_0) = \mu_T$, or $R_0 = L\sqrt{2\mu_T/\omega_T}$), is determined from the condition that the integral of the density is equal to N, $R_0 = L(15aN/L)^{1/5}$, where we have neglected the depletion [26]. Spherical symmetry reduces the integral (16) to a one-dimensional integral over the radial distance R. Finally, we substitute R by the effective chemical potential μ,

$$R = R_0\,\sqrt{1-\mu/\mu_T}. \tag{20}$$

In carrying out this substitution, we replace n_0 by μ/λ and the delta functions by

$$\delta(\omega \pm E_q) \to \delta\left(\mu - \mu_q(\omega)\right)\left|\partial E_q/\partial\mu\right|^{-1}, \tag{21}$$

where $\mu_q(\omega)$ is the effective chemical potential in the region where E_q or $-E_q$ equals ω,

$$\mu_q(\omega) = \frac{1}{2}\left[\frac{\omega^2}{q^2/2m} - \frac{q^2}{2m}\right], \tag{22}$$

and $\partial E_q/\partial\mu = q^2/2m/E_q$. The resulting expression for the dynamical structure factor is simple:

$$S_{TF}(\mathbf{q},\omega) = \begin{cases} \frac{1}{2\omega_{\rm T}}\left(\frac{R_0^3}{aL^2}\right)\frac{\mu_q(\omega)}{\mu_{\rm T}}\sqrt{1-\frac{\mu_q(\omega)}{\mu_{\rm T}}} \times \left(1+\frac{1}{\exp(\beta\omega)-1}\right) & \text{if } \omega > 0 \text{ and } 0 < \mu_q(\omega) < \mu_{\rm T} \\ \frac{1}{2\omega_{\rm T}}\left(\frac{R_0^3}{aL^2}\right)\frac{\mu_q(\omega)}{\mu_{\rm T}}\sqrt{1-\frac{\mu_q(\omega)}{\mu_{\rm T}}} \times \left(\frac{1}{\exp(\beta|\omega|)-1}\right) & \text{if } \omega < 0 \text{ and } 0 < \mu_q(\omega) < \mu_{\rm T} \\ 0 & \text{otherwise ,} \end{cases}$$

which is the main result of this paper. In Fig. 1, we show the dynamical structure factor as a function of energy transfer, for a fixed scattering angle or momentum transfer q corresponding to $q^2/2m = 0.1\mu_T$. The temperature of the condensate is different for each curve, $k_BT = 0$ (dot-dashed curve), $0.3\mu_T$ (dashed curve) and $0.5\mu_T$ (solid line). Notice that the ratio of the intensities distributed over positive and negative transfer energies, is sensitive to the temperature. Indeed, (23) satisfies the principle of detailed balance: $S(\mathbf{q},\omega) = \exp(\beta\omega)S(-\mathbf{q},-\omega)$, which is a general result [25]. This temperature dependence implies that scattering experiments can directly measure the temperature of the atomic-trap condensates simply by comparing the scattered intensities at ω and $-\omega$ energy transfer, $T = \frac{\omega/k_B}{\ln[S(\mathbf{q},\omega)/S(-\mathbf{q},-\omega)]}$.

IV. DISCUSSION OF LIMITS OF VALIDITY

Although the results of this paper are limited to dilute condensates of low depletion, the quasi-homogeneous description has a much broader range of validity. One necessary condition for the validity of the dynamical quasi-homogeneous description, is the validity of the static Thomas-Fermi model. In the low temperature region discussed in this paper, this amounts to the requirement that the size of the condensate exceeds the extent of the ground state, $R_0 >> L$, or equivalently, $\mu_T >> \hbar\omega_T$ ([14], [15], [27]). Furthermore, approximating the structure density $\sigma(\mathbf{R};\mathbf{q},\omega)$ by the value of the homogeneous system is only sensible if the spatial variations of the BEC are imperceptible in the region probed by $\sigma(\mathbf{R};\mathbf{q},\omega)$, i.e. if q $> l_v^{-1}$, where l_v is the scale on which the condensate varies spatially. For example, for a harmonic oscillator trap, we could choose $l_v \approx R_0/3$ since $\mu(\mathbf{R})$ varies by approximately 10 % from the middle of the trap to $R = R_0/3$. The resulting restriction, $q > l_v^{-1}$, requires a scattering angle larger than the scattering angle for coherent scattering $q \leq R_0^{-1}$, so that the quasi-homogeneous model is only useful in describing incoherent scattering. Finally, we note that long-time fluctations, even on short distances, are affected by the finite size effects. Roughly speaking, if a localized perturbation creates an excitation that lives long enough to propagate to a region of different density and reflect back to the position of origin, then one should describe the fluctuations in terms of discrete harmonics or eigenstates of the finite system. The quasi-homogeneous description is valid either if the lifetimes of the excitations are sufficiently small so that the reflected excitation is damped out, or, if the scattering data probe the fluctuations only over time periods less than t_v, the time needed for the reflected excitation to return. The restriction to short-time fluctuations can be achieved by using an energy resolution for the transfer energy that is less than or equal to $\Delta\omega \sim t_v^{-1}$. We estimate t_v by assuming that the wave front of the excitation propagates at the local velocity of sound, c $= \sqrt{\mu/m}$, and we equate t_v to the time necessary for the wave front to travel a distance l_v, $t_v \sim l_v/c$. In the middle of the trap, $c = \omega_T \times R_0/\sqrt{2}$, so that $t_v \sim \frac{l_v/R_0}{\omega_T}$ and thus $\Delta\omega \sim t_v^{-1} \sim \omega_T \times (R_0/l_v)$. We conclude by stating that the above considerations indicate that

the Thomas-Fermi dynamical structure factor, as a function of the energy transfer, should be interpreted as a 'smooth' version of the measured structure factor and that we should compare intensities integrated over frequency intervals larger than or equal to $\Delta\omega$. In reality, the estimate of $\Delta\omega$ depends on the region of the condensate that is probed, which in turn is determined by the value of the energy and momentum transfer. The middle of the trap, which is probed on the high–frequency side for $|\omega|$ ($|\omega|$ near $\sqrt{(\mathrm{q}^2/2\mathrm{m}+\mu_{\mathrm{T}})^2-\mu_{\mathrm{T}}^2}$) requires the lowest value of $\Delta\omega$ (estimated above), whereas on the low frequency-side, $|\omega| \sim q^2/2m$, the edge of the condensate is probed, where the quasi-homogeneous description cannot be trusted and $\Delta\omega \to \infty$.

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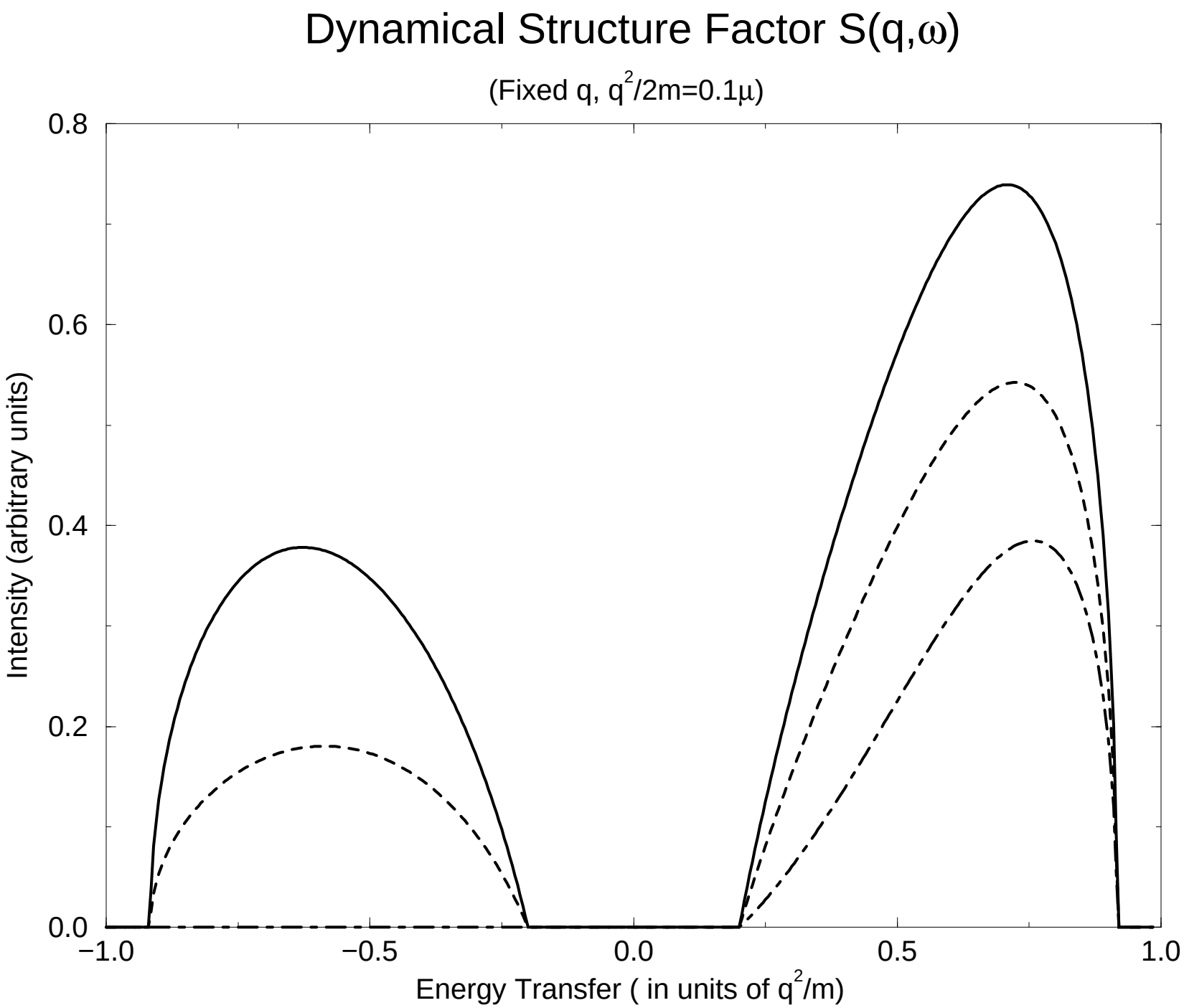
Figure Caption

Figure 1: Plots of the Thomas-Fermi dynamical structure factor as a function of the energy transfer ω, for fixed momentum transfer q, $q^2/2m = 0.1\mu_T$. The three curves show the results at different temperatures, $k_BT = 0$ for the dot-dashed line, $k_BT = 0.3\mu_T$ for the dashed curve, and $k_BT = 0.5\mu_T$ for the plot shown in solid line.


Dynamical Structure Factor S(q,ω)
(Fixed q, q²/2m=0.1μ)
Intensity (arbitrary units)
0.0
0.2
0.4
0.6
0.8
−1.0
−0.5
0.0
0.5
1.0
Energy Transfer (in units of q²/m)